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This document is the final report for AFOSR Grant F49620-01-1-0456, "Worksstation Cluster for Simulations for Quantum Lattice-Gas Automata and Entropic Lattice Boltzmann Models." Under the terms of this grant, a workstation cluster was purchased by Professor Bruce Boghosian of the Department of Mathematics at Tufts University in order to carry out large-scale simulations in support of his other AFOSR project F49620-01-1-0385, "Quantum Lattice-Gas Automata and Hydeodynamics," which was funded by AFOSR for three years, begining in 2001. This report is restricted to a description of the computer that was purchased, and to the process of purchasingit. A description on the results thus obtained will be included in the final report of AFOSR grant F49620-01-1-0385.

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Workstation Cluster for Simulations of Quantum Lattice-Gas Automata and Entropic Lattice Boltzmann Models (Final Report for AFOSR Grant Number F49620-01-1-0456)

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February 2001

Abstract

This document is the final report for AFOSR Grant F49620-01-1-0456, "Workstation Cluster for Simulations of Quantum Lattice-Gas Automata and Entropic Lattice Boltzmann Models." Under the terms of this grant, a workstation cluster was purchased by Professor Bruce Boghosian of the Department of Mathematics at Tufts University in order to carry out large-scale simulations in support of his other AFOSR project F49620-01-1-0385, "Quantum Lattice-Gas Automata and Hydrodynamics," which was funded by AFOSR for three years, beginning in 2001.

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Contents

1 Description of Project

Professor Bruce M. Boghosian of the Department of Mathematics at Tufts University is currently receiving funding under AFOSR project F49620-01-1-0385, "Quantum Lattice-Gas Automata and Hydrodynamics," to carry out large-scale simulations in support of the Quantum Computation effort at Air Force Research Laboratory at Hanscom AFB. This project has been funded for three years beginning in 2001. One of the principal areas of study is quantum lattice-gas automata as a paradigm for quantum computation. From the outset, it became clear that the project would require substantial computational facilities in order to simulate quantum lattice-gas automata.

To understand the computational requirements involved, consider a quantum lattice-gas model for diffusion in one spatial dimension. To understand this, we first describe a corresponding classical model. We suppose that we have a lattice of N sites, with up to three particles per site, each of unit mass. The three particles may be associated with negative velocity, zero velocity and positive velocity, respectively. In each time step of the model, the particles stream in the direction of their velocity to the next site, and undergo a collision. In order to simulate diffusion, the collisions should conserve mass, but not momentum. One possibility, investigated many years ago in a paper by Boghosian and Taylor [1], is to have collisions with probability p only if there are exactly two particles at the site. In the event of such a collision, the result is one of the other two two-particle states with even odds. This simple classical model was shown to have an average density $\rho \in [0, 3]$ that obeys the diffusion equation

$$\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{\partial \rho}{\partial x}\right),$$

with nonlinearity introduced by the density-dependent diffusivity [1],

$$D = \frac{1}{3}\left(\frac{2}{p\rho} - 1\right).$$

Now consider the problem of quantizing the above-described lattice-gas automaton. For simplicity, we eliminate the rest particle, and allow a nontrivial collision only when there is one particle present at a site. We suppose that the collision takes the particle to the other one-particle state for that site, or leaves it unchanged, with even odds. The system as a whole has $2N$ bits, and so it may be in any one of $2^{2N} = 4^N$ states. A quantum model will assign a complex amplitude to each of these states. The evolution of this amplitude vector will be given by the action of a $4^N \times 4^N$ unitary matrix.

The unitary matrix described above has 16^N entries. Fortunately, most of them are zero, so the matrix is sparse. A set of states with the same masses at each site constitute an equivalence class. A collision will take any state into another in the same equivalence class. The size of an equivalence class is thus 2^n, where n is the number of two-particle sites on the lattice. The number of equivalence classes of size 2^n may be found by noting that the n two-particle sites may be placed in any of $\binom{N}{n}$ configurations, and the remaining $N - n$ sites may be either zero-particle or three-particle sites for a total of 2^{N-n} possibilities. Thus, there are a total of

$$\sum_{n=0}^{N} \binom{N}{n} 2^{N-n} = (1+2)^N = 3^N$$

equivalence classes. The number of nonzero elements of the unitary matrix is then

$$\sum_{n=0}^{N} \binom{N}{n} 2^{N-n} (2^n)^2 = \sum_{n=0}^{N} \binom{N}{n} 2^{N+n} = 2^{2N} \sum_{n=0}^{N} \binom{N}{n} \left(\frac{1}{2}\right)^{N-n} = 2^{2N}\left(1+\frac{1}{2}\right)^N = 6^N.$$

The fraction of matrix elements that are nonzero is thus

$$\frac{6^N}{16^N} = \left(\frac{3}{8}\right)^N.$$

[1] There are minor corrections to the formula for the diffusivity, the origins of which are interesting and discussed in detail in the reference [1], but they are not essential to the present discussion.

The simulation of the evolution of this quantum lattice-gas automaton thus requires the ability to manipulate large sparse matrices. A single time step of this automaton for a lattice of only twelve sites will require the multiplication of complex vectors of length $4^{12} \approx 1.68 \times 10^7$ with unitary matrices of $6^{12} \approx 2.18 \times 10^9$ nonzero elements. The extension of these methods to higher dimensions, or to more complicated quantum lattice gases for fluid dynamics will thus require enormous amounts of computing ability, as well as analytic and computational techniques more advanced than those alluded to in the above discussion.

Likewise, the classical simulation of entropic lattice-Boltzmann models has also been shown [2] to require huge computational resources. Entropic lattice-Boltzmann models hold the promise of guaranteed stability for arbitrarily small viscosity. While this still does not mitigate the turbulence problem for Direct Numerical Simulation of viscous fluids, since the lattice size would still need to be large enough to resolve the smallest eddies, it may have better computational scaling than other alternatives. It may also introduce a natural kind of eddy viscosity when the smallest eddies are not resolved.

For all of these reasons, AFOSR Grant F49620-01-1-0456 requested $34,942 for the purchase of a workstation cluster for these kinds of simulations. The proposal specified a cluster of Apple G4 processors, connected by a high-bandwidth Myranet network. This was the first platform considered, and Apple loaned one such processor to the PI during the summer of 2001 for testing purposes. It performed very well in our tests using the Absoft Fortran complier. Much of our motivation was based on the successes of Decyk and his collaborators at UCLA [3]. At the same time, there was concern that the Macintosh platform was not really designed for clustering, so that software amenities such as easy-to-use message-passing libraries, and hardware amenities such as rack mounts were not available [2].

In the end, we decided to purchase a Linux cluster from Microway, Inc. This company, located in Plymouth, MA, specializes in the construction and assembly of Linux clusters. They deliver and install them preloaded with software, two-year offsite hardware warantee, and technical support for users for the lifetime of the computer. The software purchased included the Portland Group suite of Fortran compilers, along with the MPI message-passing library.

The final quote received from Microway was dated October 24, 2001. After experimenting with cost estimates for various configurations, we decided on a dual Athlon MP 1600+ (1.4GHz) cluster in 2U Rackmounts, for a total of 18 CPU's. An accounting of the hardware is given in Fig. 2. The total cost for the above list of items was thus $41,234. Of this, $34,942 came from the AFOSR grant, and the remainder was funded by Tufts University.

The machine was delivered on February 2, 2002, and Microway returned to install it on February 13, 2002. Tufts University provided a home for the machine in their main machine room in the Tufts Administration Building. This machine room houses all of the mainframes used on campus, and is equipped with air conditioning, UPS power sufficient to keep all machines running for an hour after an outage, halon fire protection, and is staffed 24/7. The extra funds and the machine room facility provided by Tufts University were a de facto, if not de jure, form of cost sharing that was not mentioned in the proposal itself.

The cluster compiled and ran a Fortran 90 program, with MPI communication, shortly after it was installed. It has been working reliably ever since. In the four months since it was installed, it was taken down only once for a planned power outage. We are still pleased with our selection of the Athlon-based Beowulf cluster, and look forward to several years of good use. We are especially pleased that the installation (both hardware and software) provided by Microway shielded us from the innumerable details involved in getting such a cluster up and working, and allowed us to remain focused on our research.

2 Conclusions

We have described the acquisition of a Beowulf computer cluster by the PI, located in the Department of Mathematics. The cluster will be used in support of AFOSR grant F49620-01-1-0385, providing mathematical and technical assistance to the Quantum Computation group at Air Force Research Laboratory at Hanscom AFB. The cluster was successfully purchased, installed, and is currently working well.

[2] Alas, for us and for them, Apple introduced rack mounts in the spring, after our purchase was made.

1. (QTY: 1) Dual Athlon MP 1600+ Master Node (4U)
   (a) Tyan S2462UNG Dual Athlon MP 1600+ CPUs w/384K Cache per CPU with AMD-760 MP chipset and 200/266MHz FSB
   (b) 5 64/32-bit PCI slots, AGP Pro 50 Slot, 2 Serial/1 Parallel/2 USB
   (c) 2GB DDR SDRAM (2 Each 1GB DDR Registered 266MHz DIMMs)
   (d) 4U 19 RackServer Chassis with 24 slide rails
   (e) 460 Watt power supply
   (f) Onboard Adaptec AIC-7899W Dual Channel Ultra3/160 SCSI Controller
   (g) 2 Each - 36GB Ultra/160 10000 RPM SCSI HDD
   (h) Sony SDT9000/BM 12/24GB Internal 4mm DAT DDS3 Tape Backup
   (i) Integrated ATI RAGE XL 4MB Video
   (j) 2 Each 3COM 3C996-T 64-bit Gigabit PCI Ethernet (TD825603)
   (k) 52X CDROM IDE Drive
   (l) 3 Floppy Drive
   (m) Red Hat Linux (CD) 7.1 with MPICH (Installed)

   Item 1 Unit Price: $5,195
   Item 1 Ext. Total: $5,195

2. (QTY: 8) Dual Athlon MP 1600+ Compute Node (2U)
   (a) Tyan S2462UNG Dual Athlon MP 1600+ CPUs w/384K Cache per CPU with AMD-760 MP chipset and 200/266MHz FSB
   (b) 5 64/32-bit PCI slots, AGP Pro 50 Slot, 2 Serial/1 Parallel/2 USB
   (c) 2GB DDR SDRAM (2 Each 1GB DDR Registered 266MHz DIMMs)
   (d) 2U 19 Rackmount Chassis with riser card with 24 slide rails
   (e) 460 Watt power supply
   (f) Onboard Adaptec AIC-7899W Dual Channel Ultra3/160 SCSI Controller
   (g) 18GB Ultra/160 10000 RPM SCSI HDD
   (h) Integrated ATI RAGE XL 4MB Video
   (i) 3COM 3C996-T 64-bit Gigabit PCI Ethernet (TD825603)
   (j) 3 Floppy Drive
   (k) Red Hat Linux 7.1 with MPICH (Installed)

   Item 2 Unit Price: $3,125
   Item 2 Ext. Total: $25,000

3. (QTY: 1) HP J1470A 15 RM Flat Panel Monitor/Kb/Mouse (TD#068181) (2U)

   Item 3 Unit Price: $2,595
   Item 3 Ext. Total: $2,595

4. (QTY: 1 Lot) Raritan MCC16 16-channel KVM Kit (2U) (Consists of: 1-MCC16, 1-RMCS16, 16-CCP20)

   Item 4 Unit Price: $2,300
   Item 4 Ext. Total: $2,300

5. (QTY: 1 EA.) 40U Microway CoolRack Cabinet (Black) (P/N 701936)
   (a) With 2 535CFM 10 fans, 4 Each 11-outlet power strips
   (b) With 1 sliding tray (for rackmountable monitor)
   (c) Cabinet Dimensions: 77.58H X 23.33W X 40.59D

   Item 5 Unit Price: $2,695
   Item 5 Ext. Total: $2,695

6. (QTY: 1) PGI Cluster Development Kit (CDK) (2 Users/64 CPUs)

   Item 6 Unit Price: $2,879
   Item 6 Ext. Total: $2,879

7. (QTY: 1 Lot) Shipping (to loading dock at Tufts University)

   Item 7 Lot Price: $570

Figure 1: Parts and Price List for Computer Cluster

References

[1] B.M. Boghosian, W. Taylor, "Correlations and Renormalization in Lattice Gases," *Phys. Rev. E* **52** (1995) 510-554.

[2] B.M. Boghosian, J. Yepez, A. Wagner, P.V. Coveney, "Entropic Lattice Boltzmann Models," *Proc. Roy. Soc. Lon.* A (2001) **457**, 717-766.

[3] V. Decyk et al., see `http://exodus.physics.ucla.edu/appleseed/appleseed.html`.

A Publications

Though publications will come from the research performed on this computer cluster, no publications were made on the acquisition of the cluster itself. The publications on the research will be described in the final report of AFOSR grant F49620-01-1-0385.

B Invited Talks and Presentations

While the PI, Professor Bruce Boghosian, gave a number of invited talks and presentations during the period of this proposal, these tended to be on the research conducted with the computer, and not on the acquisition of the computer itself. For this reason, these talks and presentations will be described in the final report of AFOSR grant F49620-01-1-0385.

C Honors and Awards

During the period of this grant, Professor Bruce Boghosian received a Visiting Fellowship from the RealityGrid project, based at Queen Mary College of the University of London. This Fellowship will enable him to visit London during the summers of 2002, 2003 and 2004, to learn and participate in the Grid Computing projects in progress there. The RealityGrid effort is aimed at using Grid Computing for problems in Materials Science. This connection may well be useful in determining future modes of operation of the machine funded by this grant; that is, at some point, we may wish to add more processors, and configure it as part of a Grid Computing network.